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FE analysis of Thermal Properties of Woven Fabric Constructed by Yarn Incorporated with Microencapsulated Phase Change Materials

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Abstract

Phase Change Materials are the substances which can store or release a large amount of energy in the form of latent heat at certain melting temperatures. Such properties open new opportunities in the development of thermo-regulating textiles for thermal protection against extreme environment. In this work, a woven fabric has been made using a novel synthetic yarn incorporated with Microencapsulated Phase Change Materials and its heat transfer property has been studied using finite element analysis. The result of simulation after post processing has been validated against experimental result. It shows a strong correlation between the predicted and experimental results. Based on validated model, delay in temperature rise as a function of time is also predicted which is not possible to be determined through experiment.

Keywords

Heat transfer, phase change material, latent heat, ABAQUS, finite element analysis, woven fabric

1 Introduction

PCMs (Phase Change Materials) possess the ability to change its physical state by absorbing or releasing heat in the form of latent heat within a certain range of temperature. Latent heat is the most efficient way of storing thermal energy and provides much higher density with a smaller temperature difference[1]. Linear chain paraffin wax such as n-octadecane is used as a phase change material for textile and clothing which has melting temperature of 28 °C closer to the human skin temperature. The phase change material is encapsulated in a polymeric shell to protect it from leakage and reduces evaporation and reaction of PCM to the outer environment. It also provides easy application on textiles without affecting the textile aesthetic properties[2]. PCMs have been applied on textiles through different techniques such as finishing, coating[3], lamination and synthetic yarn extrusion[4],[5]. PCMs are widely used as thermal energy storage systems in buildings[6], solar heating systems[7], protective nonwovens[8], fibres and fabrics[9].

The main objectives for the incorporation of PCMs in textiles are to get thermal insulation and comfort properties. PCMs possess the ability to change their state from solid to liquid or vice versa within a certain temperature range. The PCMs absorb energy during the heating process as phase change occurs and same amount of energy is being transferred to the wearer or environment during reverse cooling process[10].

Heat transfer analysis on textiles containing PCMs has been investigated by different researchers. Lamb et al[11] determined heat loss through fabrics by ventilation with and without phase change additives. They claimed that incorporation of PCMs at the proper location of layered garment can significantly enhance the insulating properties of fabrics. Pause[12] in 1995 investigated the development of heat and cold insulating membrane structures containing PCMs and claimed the substantial improvement in the thermal insulation of the material. But in their investigation, there was no numerical simulation.

Nuckols[13] established an analytical model for diver dry suit with comfortemp® foams containing MicroPCMs (Microencapsulated Phase Change Materials) and studied the thermal performance of fabric. He concluded that microencapsulated octadecane gave better thermal protection against microencapsulated hexadecane due to lower melting temperature of hexadecane. Shim et al[14] quantified the effect of PCM in clothing to investigate the thermal performance of fabric. They claimed that heating and cooling effect could last for 15 minutes depending on the number of PCM garment layers and combination of garments. Junghye et al[15] developed thermostatic fabrics treated with microcapsules containing n-octadecane and compared the thermal storage/release properties with untreated fabric.

In 2004 Ghali et al[16] experimentally and numerically investigated the effect of PCM on clothing during periodic ventilation. They claimed that heating effect could last for approximately 12.5 minutes in fabric treated with MicroPCMs depending on the amount of MicroPCMs and outdoor temperature conditions. Li and Zhu[17] developed a mathematical model of coupled heat and moisture transfer with PCMs and simulated the thermal buffering effect of PCM in fabrics. They numerically computed the temperature distribution and moisture concentration in porous textiles with and without PCM and validated their model with experimental results. Fengzhi et al[18] developed a mathematical model of heat and moisture transfer in hygroscopic textiles containing microencapsulated PCMs. They further used the model to investigate the effect of fibre hygroscopicity on heat and moisture transfer properties of textile with MicroPCMs. They claimed on the basis of results from their proposed model that fibre hygroscopicity not only has influence on the distribution of water vapour concentration in the fabrics and water content in fibres but also on the effect of MicroPCMs in delaying fabric temperature variation during environment transient periods.

In 2009, Fengzhi[19] did numerical simulation work to investigate the effect of MicroPCMs distribution on heat and moisture transfer in porous textile materials and claimed that the total heat loss from body is lowest when PCMs are located in the outer layer of fabrics. Ying et al[20] used finite difference volume method to numerically simulate the heat and moisture transfer characteristics on multilayer PCM incorporated textile assemblies. Bendkowska et al[21] studied the thermo-regulating behaviour of nonwoven incorporated with MicroPCMs and determined the amount of latent heat per unit area of nonwoven fabrics. They reported that distribution of MicroPCMs in fibrous substrate and position of PCMs layer in garments has significant effect on thermo-regulating behaviour of the garments. Alay et al[22] studied the thermal conductivity and thermal resistance of fabrics containing MicroPCMs under steady state conditions. Yoo et al[23] studied the effects of the number and positions of fabric layers coated with nanosilver nonadecane PCM in a four layer garment to investigate its thermo-regulating properties. They used Human-Clothing-Environment simulator for the evaluation of temperature changes in the air layers of microclimate within clothing. Their research showed that outer layer containing PCM in garment assembly gives good thermo-regulating properties.

In 2013, Hu et al[24] developed a mathematical model based on finite difference technique to investigate the heat flow in protective clothing embedded with PCM for fire fighters. They simulated the temperature variation by comparing different thickness and position conditions of PCM in protective clothing as well as melting phase of the PCM and human irreversible burns using one dimensional mathematical model. More recently Siddiqui and Sun[25] investigated thermal conductivity of MicroPCMs coated woven fabrics made of cotton, wool and Nomex® using finite element method. They evaluated thermal conductivity of fabrics in two steps by generating the two separate unit cell models for coating portion only and the coated composite fabrics.

The FE heat transfer analysis on PCM textiles has been reported in literature using PCM as a composite coated layer on fabric substrates mentioned above. No theoretical research work has yet been reported in the effect of heat transfer behaviour of yarns and fabrics incorporated with MicroPCM and how to inform the yarn and fabric engineering in practice. The aim of this research is to investigate the heat transfer properties of woven fabric constructed by Multifilament polypropylene yarn incorporated with MicroPCMs developed through an extrusion process by authors. A geometrical model was developed based on actual fabric, shell and core part of the MicroPCMs. The heat transfer simulation is done using finite element method under Abaqus environment. The further prediction of thermo-regulating effect on fabric based on the validated model has also been discussed in the present work.

2 Materials

In this study a plain woven fabric was developed using multifilament polypropylene twisted yarn[26]. The yarn was extruded by melt spinning technique using bench-top extruder and then twisted on a twisting machine containing 3 twists per inch (TPI). The multifilament yarn was incorporated with 4% MicroPCMs through the melt spinning process. MicroPCMs were supplied by Microtek laboratory Inc. MicroPCMs contained melamine formaldehyde as capsule shell and n-octadecane as functional core material. The properties of MicroPCMs are listed in Table 1.

Table 1 Physical Characteristics of MicroPCMs should be placed here

3 Methodology

A handloom was used to make plain woven fabric. The developed MPCM yarn was used for both warp and weft. Fabric specifications are listed in Table 2. British Standard BS 2010 was followed to determine the linear density of yarn. For the confirmation of incorporated MicroPCMs in yarn, DSC (Differential Scanning Calorimetry) 12E and SEM (Scanning Electron Microscopy) Hitachi S-4300 were used. Microscopic images were used to study the geometry of woven fabric. Fabric thickness was measured using Fabric Assurance by Simple

Testing (FAST) instrument FAST-1 under 2gf/cm^2. Unit cell was created based on the studied geometries of the fabric.

Table 2 Dimensions of fabric geometric model should be placed here.

3.1 Calculating number of Capsules

For calculation of the number of capsules within the yarn, it was important to determine the length of straight yarn. The length of yarn in woven fabric is difficult to determine because of the crimp in the yarn. Therefore a method was developed to determine the length of yarn in a unit cell of woven fabric as shown in Figure 1. Furthermore number of capsules was calculated for realistic modelling on the basis of yarn length.

Figure 1 Determination of crimped yarn length should be placed here

Length of the yarn of a repeat unit can be calculated by:

$$L = S_1 + \ell^{/} + S_2 + \ell^{//} + S_3 \qquad (1)$$

where L is the total length of a single yarn in a unit cell and $\ell^{/}$, $\ell^{//}$ are the straight portion of yarn, the arc length S can be calculated by using the relation

$$S = r\alpha \qquad (2)$$

where r is the radius of the circular loop and α is the angle of arc. Based on this length, the volume of yarn was calculated and number of capsules within the yarn against the percentage was obtained accordingly.

The above developed method is validated through ImageJ analysis as shown in Figure2. The correlation between the predicted length by numerical method and result from ImageJ was found to be 98.62% showing very close agreement. The values calculated from numerical method and ImageJ software has been shown in Table 3.

Figure 2 Crimped yarn length through Image Analysis should be placed here

Table 1 Validation of length of crimped yarn should be placed here

3.2 Calculation of thickness of encapsulating shell

For geometric model of MPCMs, the shell thickness of microcapsule was calculated using the following equation[27].

$$T = R\left(1 - \sqrt[3]{\frac{P \times \rho_S}{\rho_C - P \times \rho_C + P \times \rho_S}}\right) \quad (3)$$

where T is the thickness of shell, R is the radius of capsule, P is the content of core material, ρ_c is the density of core material and ρ_s is the density of solid shell material.

And the content of the core material can be found by using the following relation[28]:

$$\text{PCM core Content } \% = \frac{\Delta \text{Hcap}}{\Delta \text{Hpcm}} \times 100 \quad (4)$$

where ΔHcap is enthalpy of MicroPCMs and ΔHpcm is the enthalpy of phase change material (core material).

3.3 Experimental study of fabric thermal property

The heat flux of the fabric was tested using an in house developed heat transfer instrument[25]. The main components consist of hot and cold plates, a heater, a heat flux sensor and a fan heat sink as shown in Figure 3. The fabric sample under investigation is placed between cold and hot plate where the lower hot plate heated by a controlled heater. Thermocouples are attached to the plates which sense and monitor the temperature (T_1) and (T_2). The difference of hot and cold plates temperatures allow the heat to transfer through the fabric sample. The heat flux sensor is attached to the upper plate and cooled by fan heat sink and gives the value of heat flux by dividing the value on multi-meter with flux sensor's sensitivity.

Figure 3 Experimental setup should be placed here

3.4 Latent heat phenomenon of MPCM fabric

Heat transfer through conduction follows Fourier's law of heat conduction which is described in equation 5.

$$H = k\frac{\Delta T}{\Delta x} \tag{5}$$

H is the heat flux, *k* is the conductivity, Δx is the thickness of the material and ΔT is the temperature gradient.

The heat transfer mechanism can be explained in a model as described in equation 6[29].

$$\int_{V_0}^{V} \rho U dV = \int_{S_0}^{S} q dS + \int_{V_0}^{V} r dV \tag{6}$$

Equation 6 is the basic energy balance for heat transfer where *V* is a volume of material with surface area *S*, ρ is the density of the material, *U* is the internal energy, *q* is the heat flux per unit area flowing into the body and *r* is the heat supplied externally into the body per unit volume.

The above relation is usually written in terms of specific heat as mentioned below:

$$c(t) = \frac{dU}{dt}$$

For latent heat where phase changes involved, the effect is shown in terms of solidus and liquidus temperature indicating area under the curve as latent heat shown in Figure 4. The line showing specific heat is linear over the temperature gradient where as in case of phase change materials the curve makes peak between solidus and liquidus temperature to store energy in terms of latent heat. The area under the curve with blue shaded region is the amount of latent heat or stored energy during phase change.

Figure 4 Principle of phase change should be placed here

4 Finite Element Simulation

4.1 Geometrical Model

Geometric model of woven fabric incorporated with MicroPCMs was developed for heat transfer analysis using finite element method. For geometric model generation, TexGen was used and 3D model was developed. The model was then exported to ABAQUS, commercial software of Dassault Simulia Corp. for finite element analysis. The geometric model contains the following parts:

- a unit cell of woven fabric which was modelled in TexGen and exported to Abaqus CAE;
- MicroPCM consisting of inner part core and outer part solid shell; and
- air to fill the gaps among the yarns.

The geometric model parts have been shown in Figure 5 which consists of yarn, MicroPCMs and air. The magnifying and cross section image of MicroPCM has been shown in the Figure 5. The green part shows the core part which comprising of PCM while the encapsulating shell part has been shown in dark peach colour.

Figure 5 Geometric model should be placed here

4.2 Material Properties and Interaction

For heat transfer analysis in ABAQUS, the material properties for each part thermo-physical properties like specific heat, conductivity etc. have been given. The complete geometric model comprises of four materials including air, yarn (polypropylene), capsule (melamine formaldehyde) and phase change material (n-octadecane). The material properties used for modelling are stated in Table 4.

Table 2 Thermo-physical properties of Materials should be placed here

For finite element analysis the following assumptions were taken:

- yarn is considered as uniform;
- effect of radiation is neglected due to small gradient of temperature;
- effect of convection is neglected; and
- no change in PCM density over change in temperature;

For simulation purpose all different parts brought together to make a single part model. For the purpose, interaction among all different parts created by merging them into a single part to induce thermal contact.

4.3 Model discretisation and boundary conditions

Four-node linear tetrahedral DC3D4 was used for meshing the model and the mesh density with 1387523 elements was obtained. The initial condition was used for the whole model and boundary condition was assigned to the one side of the fabric as done in real experiment. The sides of the fabric were considered as completely insulated. Two temperature boundary conditions are used as follow:

$T_{(1)} = T_1$

$T_{(2)} = T_2$

T_1 is the initial temperature of the fabric while T_2 is the boundary temperature of the fabric.

5 Results and Analysis

Figure 6 shows the simulation results heat flux contour and temperature contour values.

Figure 6 Heat flux and temperature contour should be placed here

Figure 7 shows the translucent visualization of fabric model after simulation. The model is shown as a single part containing MicroPCMs inside distributed randomly. The magnified image shows the heat transfer through the fabric and MicroPCMs.

Figure 7 Visualization of fabric model containing MPCM should be placed here

Table 5 shows the heat flux values obtained experimentally and predicted from post processing in Abaqus. The agreement between the two is 91.02% which shows that the model is validated and can be used for further investigation of heat transfer characteristics of MicroPCM fabric. The methodology adopted in the model can be used to analyse heat transfer of different textiles incorporated with MicroPCMs and fabrics containing different amount of MicroPCMs.

Table 3 Result comparison between FE model and experiment should be placed here

Figure 8 shows the cut view of fabric with and without MicroPCMs from z-axis at time interval t= 2000sec for both fabrics with and without MicroPCMs. The temperature where MicroPCMs are not present, reaches around 39 °C, while the temperature in fabric containing phase change materials reaches around 27 °C which enables the thermo-regulating effect of MicroPCMs within the textiles.

Figure 8 Cut view of Fabrics with and without MicroPCMs from Z-axis will be placed here

6 Time dependent thermo-regulating effect

PCMs around their melting point start melting and store energy in the form of latent heat. The constant supply of heat does not allow the temperature to rise near the melting point of PCM and increase in temperature delays for certain period of time depending on the amount of PCMs used. This delay in temperature increment characteristic of PCMs as a function of time is impossible to be determined through experiment. This thermo-regulating property has been predicted from ABAQUS using post processing based on the validated model.

Figure 8 shows the time dependent temperature change for the three fabrics without MPCM, with 4% MPCM and with 10% MPCM. Overall the temperature increases as the time increases. However for the MPCM containing fabrics, near the melting temperature of PCM the graph proceeds linearly with time allows storing latent heat and resulting in the delay in the increase of temperature. It also shows that as the amount of PCM increases in the fabric from 4% to 10%, the thermo-regulating effect is enhanced and covered a longer period of time.

Figure 9 Thermo-regulating effect vs time will be placed here

7 Implications and limitations of the FE model

The present model can be used for any types of synthetic fabric incorporated with MicroPCMs such as polyester, nylon, acrylic etc. Besides the assumptions made for the model generation, the limitation of FE model also lies in that the present model cannot be used for different geometry other than plain weave. For other woven structures the models need to be re-validated by experimental results. Any properties for prediction can then be studied and analysed based on the validated models.

8 Conclusions

The geometry of yarn and woven fabric with and without MicroPCMs have been studied and the three dimensional models were developed for finite element analysis. The heat transfer of woven fabric incorporated with MicroPCMs was successfully investigated using Abaqus. The agreement between the heat flux predicted through finite element method and obtained experimentally was found 91.02%. Based on this validated model the time dependent thermo-regulating effect is studied which shows that as the amount of PCM in the fabric increases, the functional characteristic of PCM increases and this enhances the thermo-regulating effect to cover a longer period of time.

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Table 4Physical Characteristic of MicroPCMs

Properties of MPCMs	
PCM	n-octadecane (C_{18})
Capsule Material	Melamine Formaldehyde
Particle size (µm)	17-20
Melting Point (°C)	28.2
Latent heat (KJ/Kg)	170-190

Table 5 Dimensions of fabric geometric model

Dimensions for Geometric Model	
Warp/Weft major axis (mm)	0.366

Warp/Weft minor axis (mm)	0.299
Fabric thickness (mm)	0.86
Total width of unit cell (mm)	0.86
Total length of unit cell (mm)	2.73
Unit cell volume (mm^3)	2.019

Table 6 Validation of length of crimped yarn

Numerical Method	ImageJ	Relative Error
3.0514 mm	3.094 mm	1.38%

Table 7 Thermo-physical properties of Materials

Property	n-octadecane	Melamine Formaldehyde	Polypropylene
Density (kg/m^3)	777	1500	910

Specific heat (KJ/Kg °K)	1.9	1.2	1.925
Thermal conductivity (W/m°K)	0.3	0.5	0.137
Latent heat of fusion (KJ/Kg)	238		

Table 8 Result comparison between FE model and experiment

Obtained from experiment (W/m^2)	Predicted from simulation (W/m^2)	Relative Error (%)
583.33	635.70	8.98%

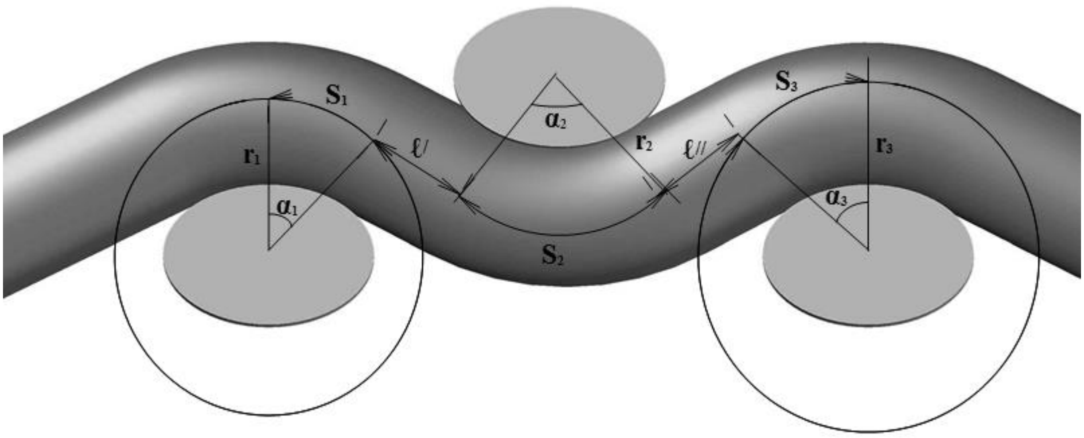

Figure 10 Determination of crimped yarn length

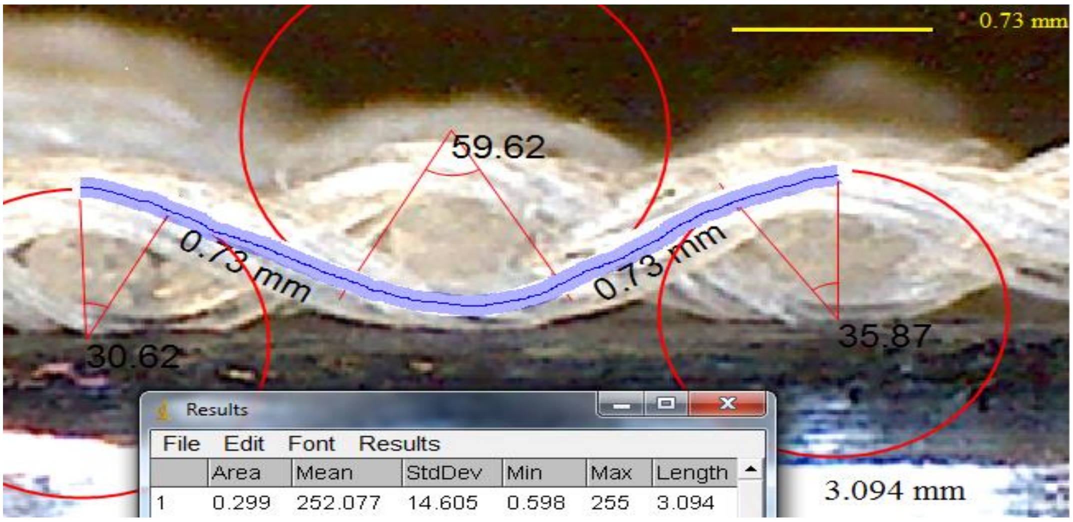

Figure 11 Crimped yarn length through Image Analysis

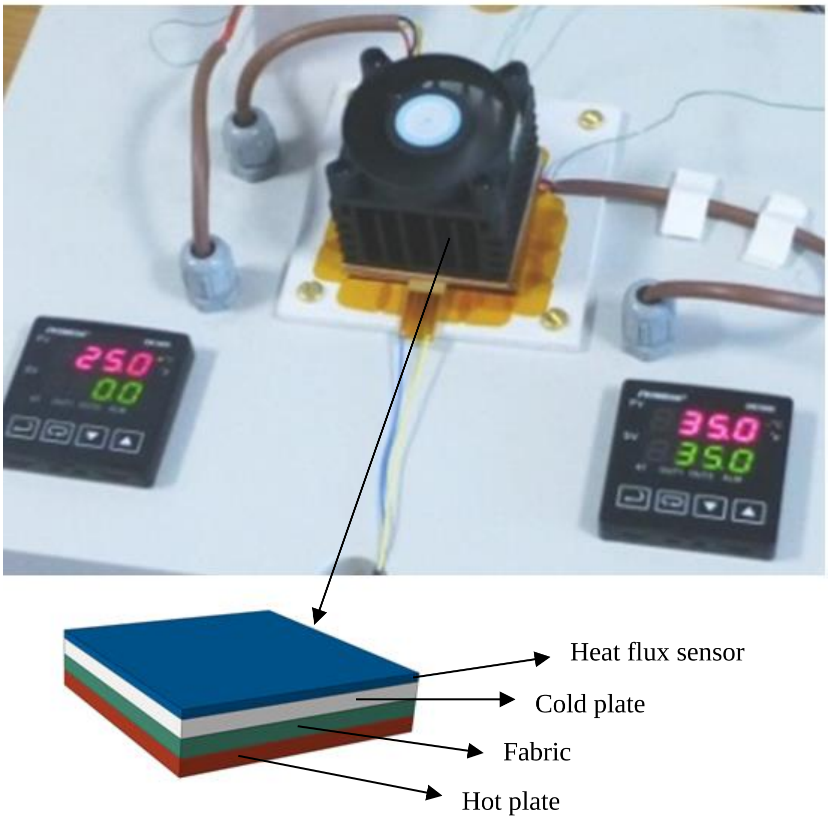

Figure 12 Experimental setup

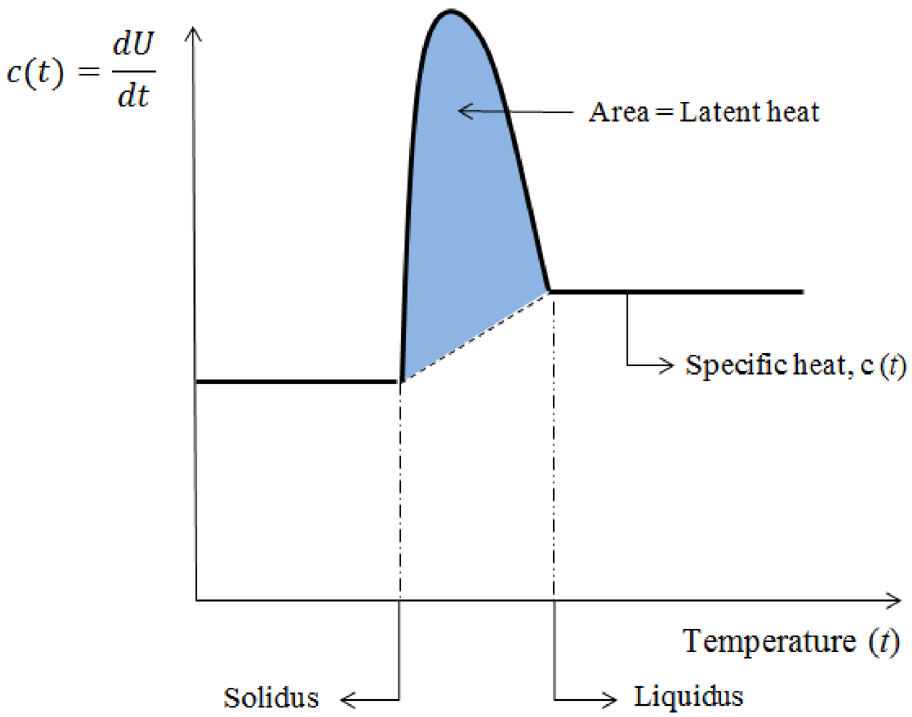

Figure 13 Principle of phase change

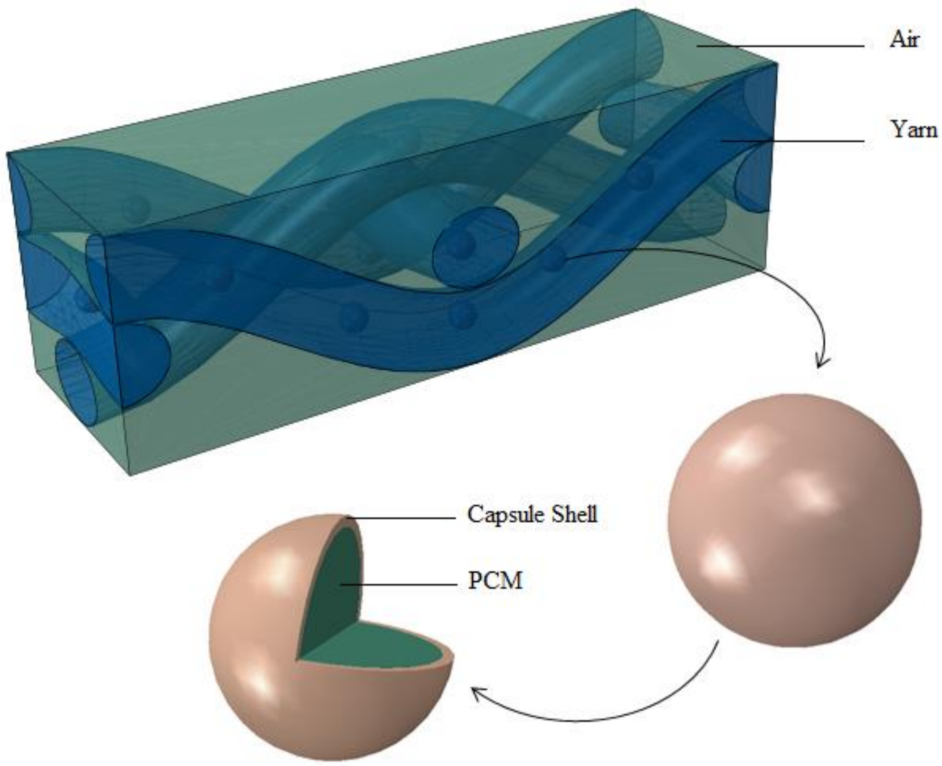

Figure 14 Geometric model

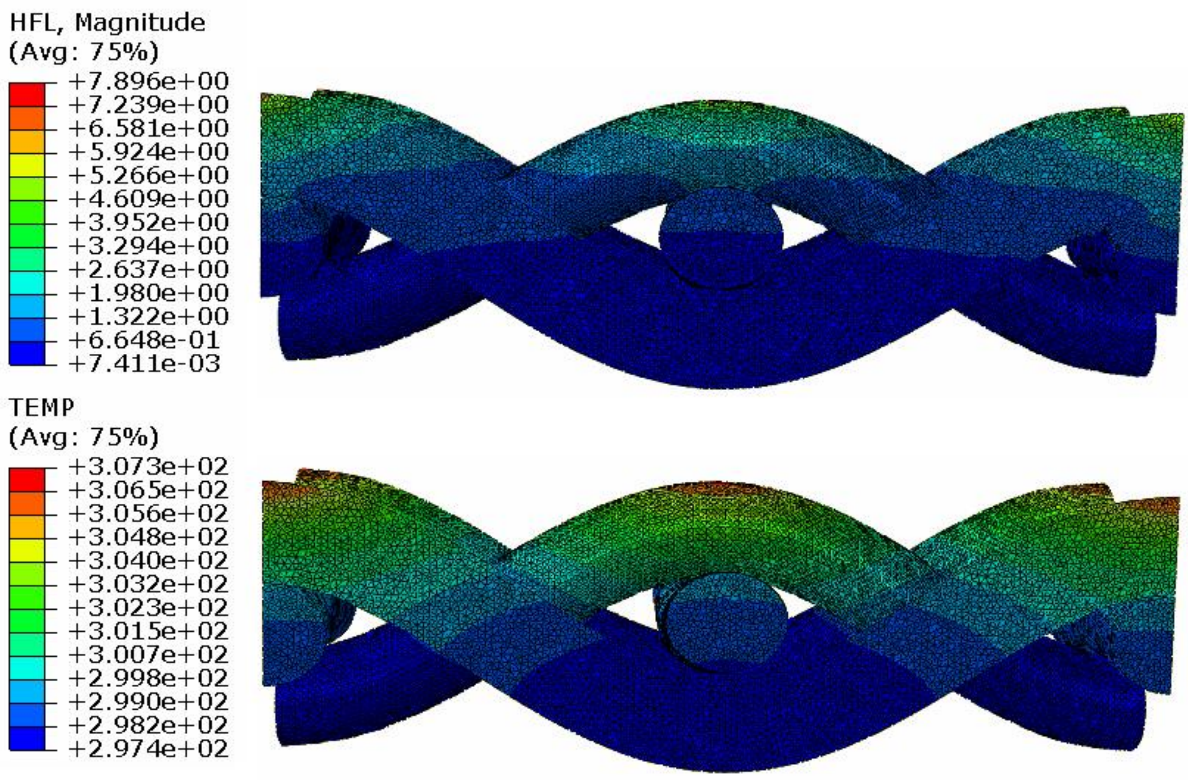

Figure 15 Heat flux and temperature contour

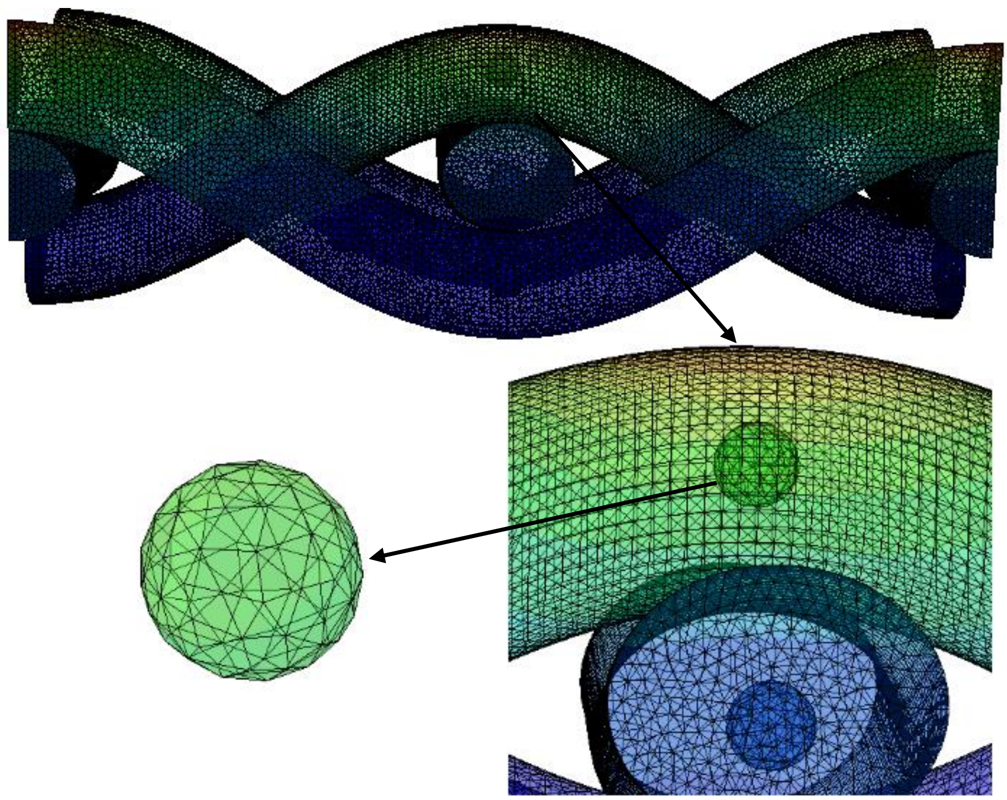

Figure 16 Visualization of fabric model containing MPCM

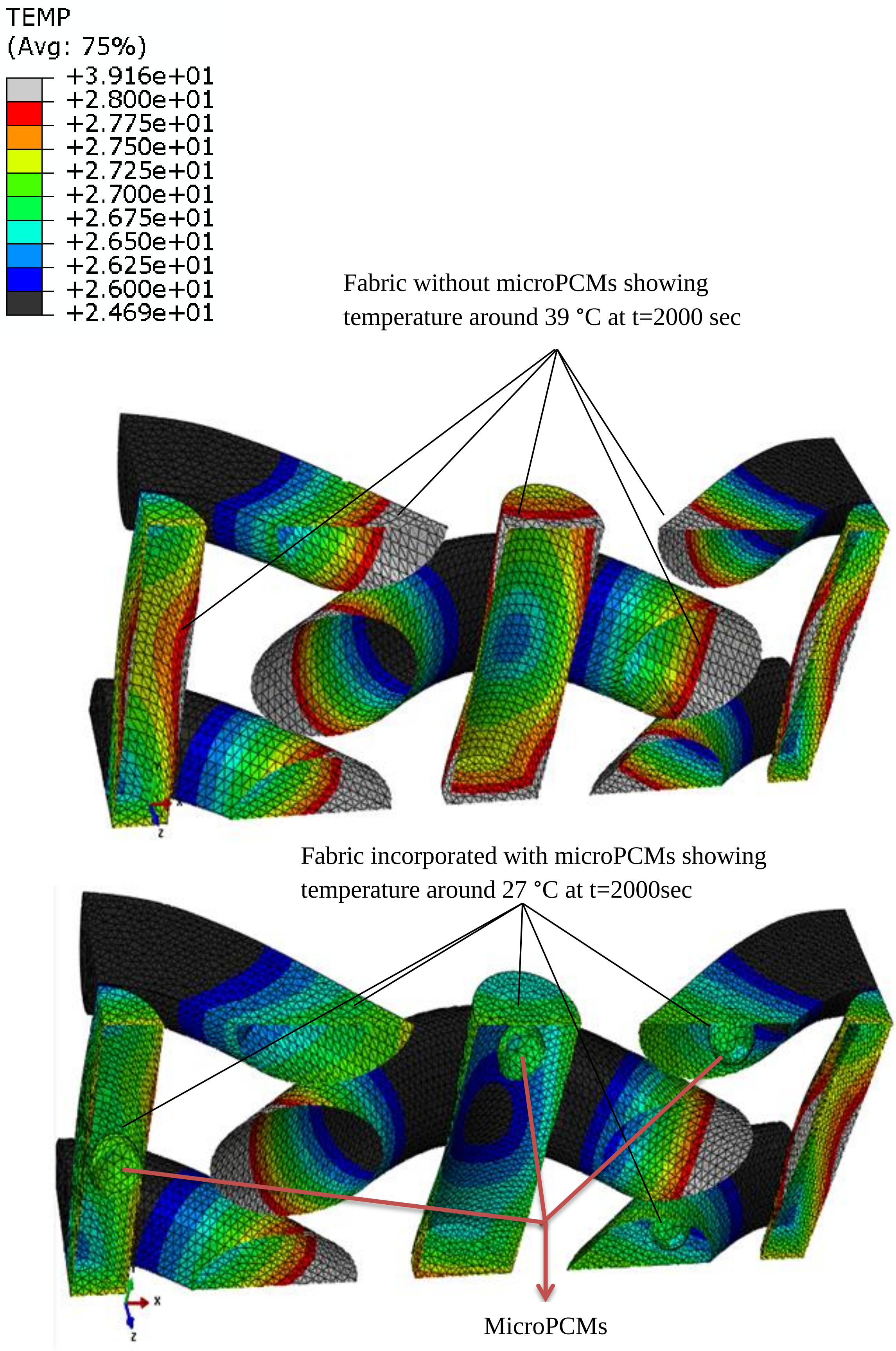

Figure 17 Cut view of Fabrics with and without MicroPCMs from Z-axis

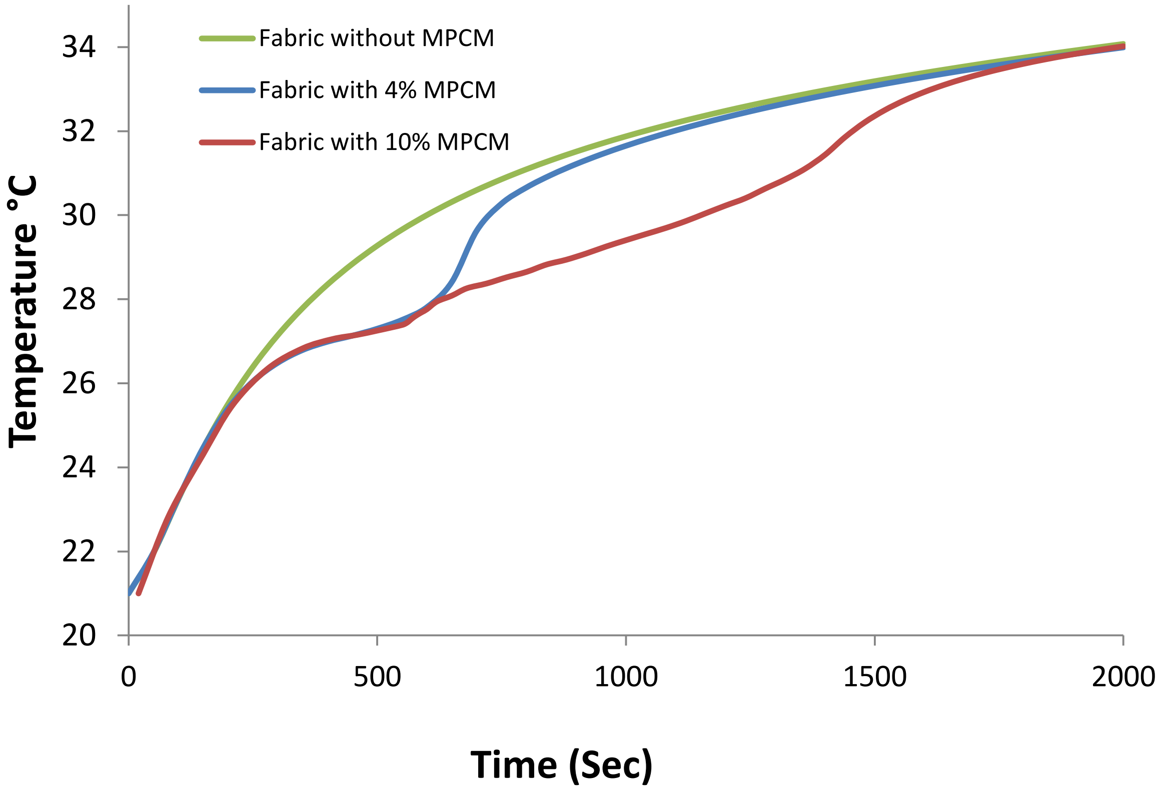

Figure 18 Thermo-regulating effect vs time